Table S1

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| CYP2C9 | | | RMSD from 1OG5 (Å) | FeO-C7 (Å)1 | rmr score | |
| Total2 | FeO-C73 |
| 1OG5  Docked con.  WT  R144C  I359L  L90P | | | 0  0  1.609  1.452  1.274  1.672 | 10.58  3.12  3.30  4.46  4.85  3.56 | 6.258  -3.032  -29.717  -28.009  -37.040  -29.591 | 0  -0.389  -0.571  0.023  0.057  -0.382 |
|  |